Clopper-Pearson Bounds from HEP Data Cuts*

Bernd A. Berg

Department of Physics, The Florida State University, Tallahassee, FL 32306, USA.

E-mail: `berg@hep.fsu.edu`

October 20, 2000

Abstract

For the measurement of N_s signals in N events rigorous confidence bounds on the true signal probability p_{exact} were established in a classical paper by Clopper and Pearson [Biometrica 26, 404 (1934)]. Here, their bounds are generalized to the HEP situation where cuts on the data tag signals with probability P_s and background data with likelihood $P_b < P_s$. The Fortran program which, on input of P_s, P_b, the number of tagged data N^Y and the total number of data N, returns the requested confidence bounds as well as bounds on the entire cumulative signal distribution function, is available on the web. In particular, the method is of interest in connection with the statistical analysis part of the ongoing Higgs search at the LEP experiments.

1

1 Introduction

The general theory of confidence bounds (or fiducial intervals) was developed by Fisher [1], Neyman and Pearson [2]. We consider a particular problem which is of interests when cuts are used to analyze high energy physics data. Typically, a neural network or some other method of performing the cuts results in probabilities (efficiencies) to tag signals more likely than background events. For instance by means of Monte Carlo (MC) simulations, these probabilities can normally be calculated. Let P_s be the probability to tag a signal and P_b be the likelihood to tag a background event, $0 < P_b < P_s < 1$. Out of a total number of N data one gets in this way

$$N^Y \quad \text{tagged data.} \tag{1}$$

It is easy to find from this the mean expectation for the signal probability. Assume that there are N_s signals and N_b background events in the data. Then we have

$$N = N_s + N_b \quad \text{and} \quad N^Y = P_s N_s + P_b N_b$$

and these two equations solve for

$$p_{\text{mean}} = \frac{N_s}{N} = \frac{N^Y - P_b N}{N (P_s - P_b)} \; . \tag{2}$$

The question is, what are the implied confidence limits on the signal probability?

The special case $P_s = 1$ and $P_b = 0$ (sure signal detection) has been treated by Clopper and Pearson [3] in 1934. After briefly reviewing their approach in the next section, we derive and illustrate the general case in section 3. This is, in part, based on Ref.[4]. In particular, the method is valid when the number of tagged data is small and returns the probability P_0 for the case that there is no signal, i.e. that the exact signal probability is $p_{\text{exact}} = 0$. This is of interest for the statistical analysis of the ongoing Higgs search at LEP [5]. Discovery of the Higgs particle on the 5σ level would mean $P_0 \leq 0.287 \, 10^{-6}$. Subsection 3.3 explains the use of the corresponding Fortran programs and how to download them from the web. Conclusions follow in the final section 4.

2 The Clopper–Pearson Confidence Limits

Let p be the likelihood that a data point is a signal. For N measurements the probability to observe k signals is given by the binomial coefficient

$$b_N(k,p) = \binom{N}{k} p^k q^{N-k} = \frac{N!}{k!\,(N-k)!}\, p^k q^{N-k} \quad \text{with} \quad q = p - 1 \ . \tag{3}$$

The probability to observe $k \geq N_s$ signals is given by

$$P_{k \geq N_s}(p) = \sum_{k=N_S}^{N} b_N(k,p) \tag{4}$$

and the probability to observe $k \leq N_s$ signals by

$$P_{k \leq N_s}(p) = \sum_{k=0}^{N} b_N(k,p) \ . \tag{5}$$

For $N = 26$ and $N_s = 10$ the functional forms of $P_{k \geq N_s}(p)$ and $P_{k \leq N_s}(p)$ are depicted in figure 1.

Assume that N_s signals are found in N measurements and that a probability $Q^c < 0.5$ (typical values are $Q^c = 0.16$ or $Q^c = 0.025$) is given. We can solve equation (4) for
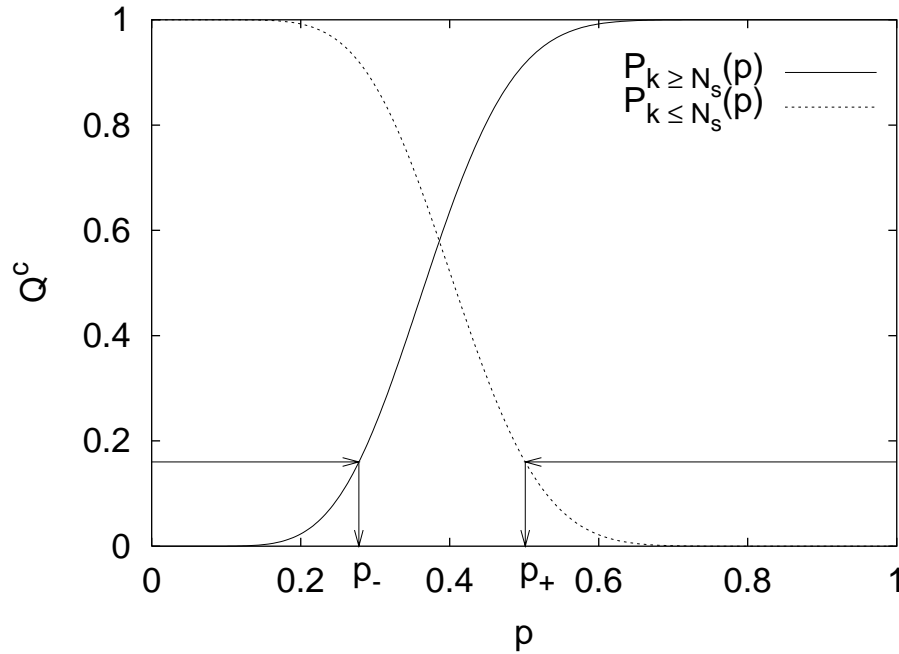

Figure 1: The probability functions $P_{k \geq N_S}(p)$ to observe $k \geq N_s$ signals in N events (4) and $P_{k \geq N_S}(p)$ to observe $k \leq N_s$ signals in N events (5) are depicted for $N = 26$ and $N_s = 10$. Symmetric 68% confidence bounds ala Clopper-Pearson are also indicated.

$P_{k \geq N_s}(p_-) = Q^c$ and p_- is a lower bound on the true signal probability p_{exact}, such that the likelihood to find $k \geq N_s$ signals in N measurement is smaller than Q^c for every $p_{\text{exact}} < p_-$. Correspondingly, we can solve equation (5) for $P_{k \leq N_s}(p_+) = Q^c$ and p_+ is an upper bound on the true signal probability p_{exact}, such that the likelihood to find $k \leq N_s$ signals in N measurement is smaller than Q^c for every $p_{\text{exact}} > p_+$. Together, this combines into the Clopper–Pearson bounds: The probability to find the true signal probability in the range

$$p_- \leq p_{\text{exact}} \leq p_+ \quad \text{is larger or equal to} \quad P^c = 1 - 2Q^c \ . \tag{6}$$

In more details the meaning of the inequality is discussed in [4]. For $P^c = 0.68$ ($Q^c = 0.16$) the $p^{\pm}$ values are indicated in figure 1. Approximately, this range corresponds to the confidence of a 1σ error bar. Similarly the confidence range corresponding to a 2σ error bar, etc., can be found.

3 Confidence Limits from Data Cuts

We are interested in the situation where signal and background data can no longer be distinguished unambiguously. Instead, a neural network or other device yields statistical information by tagging signals with efficiency P_s and background data with probability P_b, as discussed in the introduction.

Applying the cuts to all N data results in N^Y tagged data ($0 \leq N^Y \leq N$), composed of $N^Y = N_s^Y + N_b^Y$, where N_s^Y is the number of tagged signals and N_b^Y is the number of tagged background data. Of course, the values for N_s^Y and N_b^Y are not known. Our task is to determine confidence limits for the signal probability p from the sole knowledge of N^Y. We proceed by writing down the probability density of N^Y for given p and, subsequently, generalizing the Clopper-Pearson method.

First, assume fixed N_s. The probability densities of N_s^Y and N_b^Y are binomial and thus the probability density for N^Y is given by the convolution

$$P^Y(N^Y | N_s) = \sum_{N_s^Y + N_b^Y = N^Y} b_{N_s}(N_s^Y, P_s) \, b_{N_b}(N_b^Y, P_b), \ N_b = N - N_s \ . \tag{7}$$

Proof: For a signal event the probability to be tagged is P_s, so $b_{N_s}(N_s^Y, P_s)$ is the probability to tag N_s^Y out of the N_s signals. Similarly, the probability for a background event to become tagged is P_b and $b_{N_b}(N_b^Y, P_b)$ is the probability to tag N_b^Y of the $N_b = N - N_s$ background events. As these two probabilities are independent, the likelihood that precisely

N_s^Y of the signals and N_b^Y of the background events are tagged becomes the product $b_{N_s}(N_s^Y, P_s) \, b_{N_b}(N_b^Y, P_b)$. Summing over all possibilities which add up to $N_s^Y + N_b^Y = N^Y$ gives the result.

Summing over N_s in (7) removes the constraint of fixed N_s and, with N, p fixed, the probability to tag k events becomes

$$b_N^Y(k, p) = \sum_{N_s=0}^{N} b_N(N_s, p) \, P^Y(k|N_s) \; . \tag{8}$$

Fourier transformation of the convolution (7) allows for an efficient numerical calculation of the $P(k|N_s)$ coefficients. In analogy with equations (4) and (5) we find the probabilities to tag $k \geq N^Y$ and $k \leq N^Y$ events to be

$$P_{k \geq N^Y}^Y(p) = \sum_{k=N^Y}^{N} b_N^Y(k, p) \quad \text{and} \quad P_{k \leq N^Y}^Y(p) = \sum_{k=0}^{N^Y} b_N^Y(k, p) \; . \tag{9}$$

For $N = 35$, $N^Y = 12$, $P_s = 0.8$ and $P_b = 0.05$ the functions [6] $P_{k \geq N^Y}^Y(p)$ and $P_{k \leq N^Y}^Y(p)$ are depicted in figure 2. The 68% confidence range (6) is also indicated in figure 2, where the
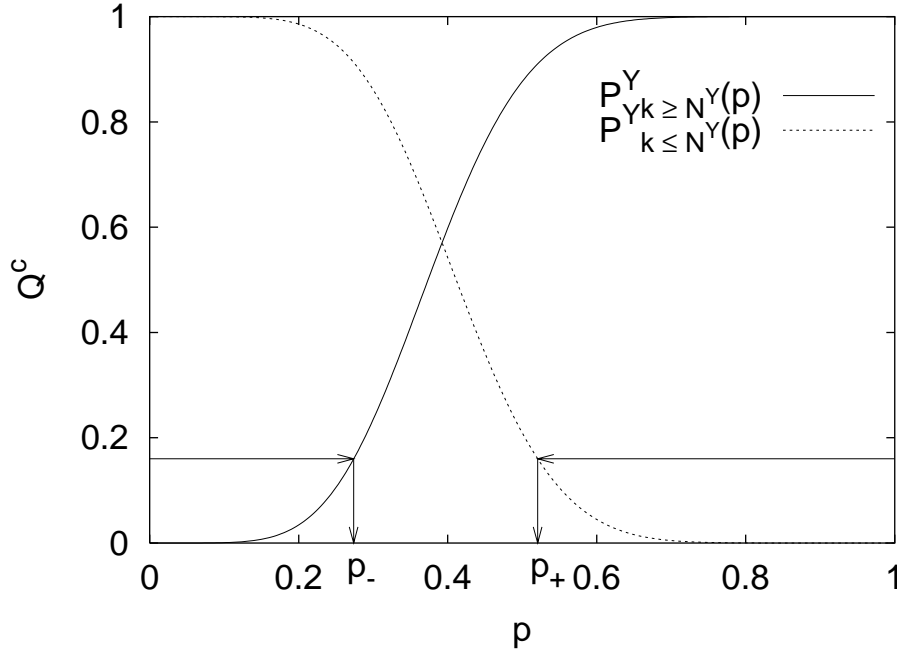

Figure 2: The probability functions $P_{k \geq N_Y}^Y(p)$ to find $k \geq N^Y$ tags in N events and $P_{k \leq N^Y}^Y(p)$ to find $k \leq N^Y$ tags in N events (9) are depicted for $N = 35$, $N^Y = 12$, $P_s = 0.8$ and $P_b = 0.05$. Symmetric 68% confidence bounds, found for $p_- = 0.274$ and $p_+ = 0.521$, are also indicated.

bound values $p_\pm$ are now defined as solutions of the equations

$$Q^c = P^Y_{k \geq N^Y}(p_-) \ \ \text{and} \ \ Q^c = P^Y_{k \leq N^Y}(p_+) \ . \tag{10}$$

The range $[p_-, p_+]$, obtained with $Q^c = 0.16$, guarantees the standard one error bar confidence probability of 68% for every true signal probability p_{exact}. For almost all values the actual confidence will be better. However, the bounds cannot be improved without violating the requested confidence probability for the case that p_{exact} happens to agree with either p_- or p_+. In the same way, bounds calculated with $Q^c = 0.023$ ensure the standard two error bar confidence level of 95.4% or better, and so on.

3.1   Data Sets with Few Signals

As outlined, data sets with few signals are of of particular interest in high energy physics. Let us replace $N^Y = 12$ of figure 2 by $N^Y = 3$. The resulting graph is depicted in figure 3. From the $P^Y_{k \geq N^Y}(p)$ curve we read off the finite probability $P_0 = 0.254$ for the likelihood that the true signal probability $p_{\text{exact}} = 0$ generates $k \geq N_y$ tags. Due to this probability the
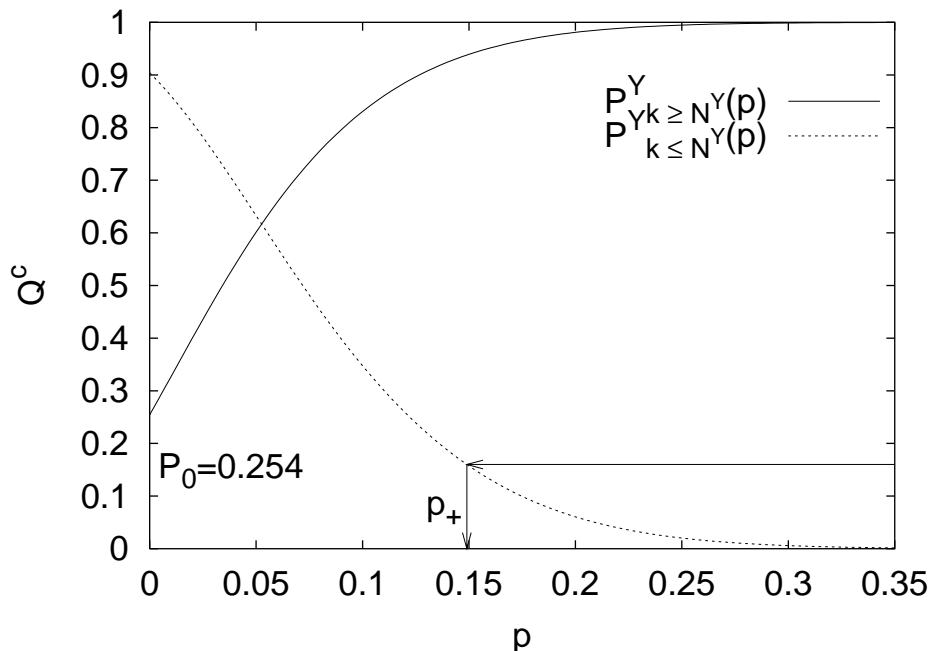

Figure 3: The same functions as in figure 2 are depicted, but for $N^Y = 3$ instead of $N^Y = 12$ tags. The lower 68% confidence bound does not exist anymore, instead the likelihood for $p_{\text{exact}} = 0$ has become $P_0 = 0.254$. The upper 68% confidence bound is found at $p_+ = 0.149$.

6

lower 68% confidence bound p_- disappears, whereas the upper p_+ bound does still exist. In passing let us note that for the data of figure 2 we have $P_0 = 0.69 \, 10^{-7}$, i.e. there $p_{\text{exact}} = 0$ is ruled out on the 5σ level.

3.2 Signal Probability Distributions

To avoid frequentist objections, the cumulative signal distribution function $F(p)$ is, in the opinion of the author, best defined as the *expectation of the researcher* to find the true signal probability p_{exact} in the range $0 \leq p_{\text{exact}} \leq p$. Our approach allows to estimate upper and lower bounds for the cumulative signal distribution function

$$F(p) = \int_{-\infty}^{p} dp' \, f(p') \quad \text{where} \quad f(p') \quad \text{is the signal probability density.} \tag{11}$$

Equation (10) implies

$$F_1(p) = 1 - P_{k \leq N^Y}^Y(p) = \sum_{k=N^Y+1}^{N} b_N^Y(k,p) \; \leq \; F(p) \; \leq \; F_2(p) = P_{k \geq N^Y}^Y(p) = \sum_{k=N^Y}^{N} b^Y(k,p) \tag{12}$$
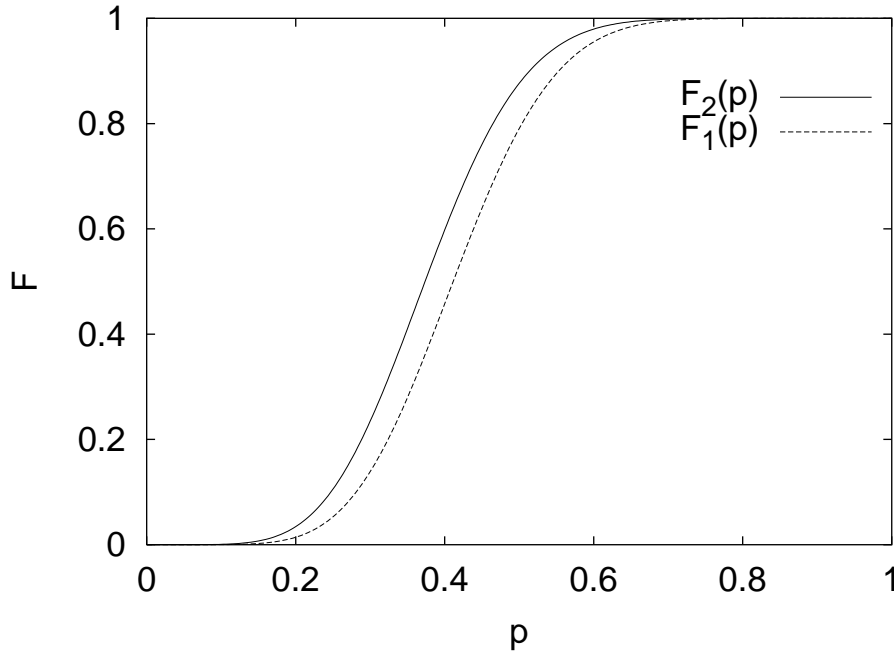

Figure 4: Upper and lower bounds, $F_2(p)$ and $F_1(p)$, for the cumulative signal distribution function $F(p)$. The values used for N, N^Y, P_s and P_b are identical with those of figure 2.

and note that $F(0) = F_2(0)$. Figure 4 shows the result for the same data which were used in figure 2. Any reasonable Bayesian estimates (which involves additional *a-priori* assumptions) should give a function $F(p)$ which is sandwiched between $F_1(p)$ and $F_2(p)$.

It is instructive to define peaked distribution functions [7] by

$$F_i^{\text{peaked}}(p) = \begin{cases} F_i(p) & \text{for} \quad F_i(p) \leq 0.5 \quad \text{and} \\ 1 - F_i(p) & \text{for} \quad F_i(p) \geq 0.5, \end{cases} \qquad (i = 1, 2) \ . \tag{13}$$

Using the same data as in figure 4, $F_1^{\text{peaked}}(p)$ and $F_2^{\text{peaked}}(p)$ are depicted in figure 5. The advantages of using peaked distribution functions instead of conventional cumulative distribution functions are:

1. The ordinate becomes enlarged by a factor of two.

2. The estimated medians are located at the peaks and the probability content of the distribution is instructively displayed.

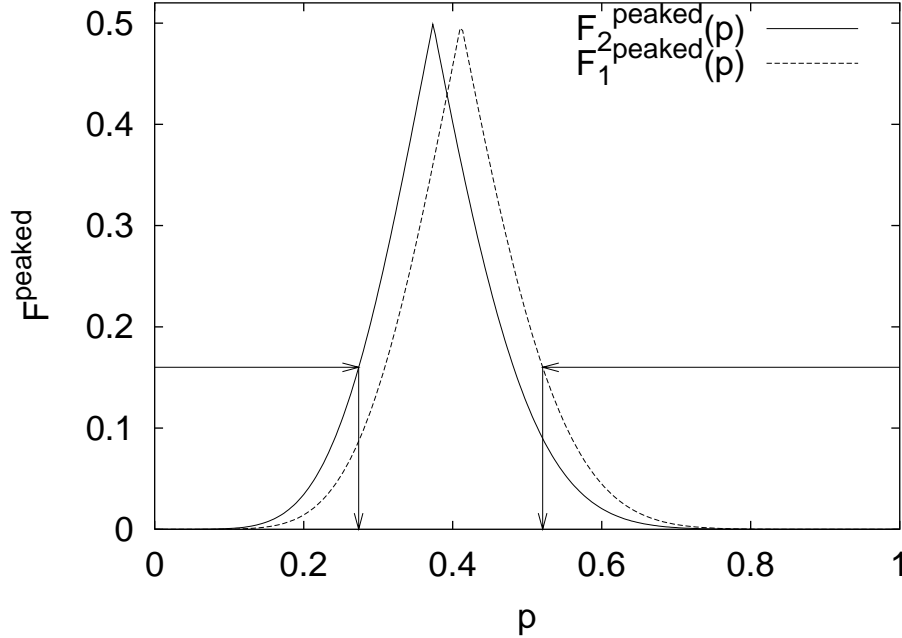3. Bounds like those of figure 1 are easily read off.

Figure 5: Peaked distribution functions $F_2^{\text{peaked}}(p)$ and $F_1^{\text{peaked}}(p)$ as defined in equation (13). The values used for N, N^Y, P_s and P_b are identical with those of figures 2 and 4.

The probability densities corresponding to the cumulative distribution functions (12) are the derivatives of the $F_i(p)$ with respect to p

$$f_i(p) = \frac{dF_i(p)}{dp} \quad (i = 1, 2) \ . \tag{14}$$

Their numerical calculation is straightforward when analytical expressions for the derivatives of the binomial coefficients in equation (8) are used. Figure 6 exhibits the results for $f_1(p)$ and $f_2(p)$ corresponding to $F_1(p)$ and $F_2(p)$ of figure 4. At $p = 0$ the probability densities have δ-function contributions

$$f_i(p) = F_i(0)\,\delta(p) + ... \ , \quad (i = 1, 2) \ . \tag{15}$$

In case of figure 6 the $F_i(0)$ coefficients are practically zero. However, for the probability densities corresponding to figure 3 there would be a substantial contribution: $F_1(0) = 0.096$ and $F_2(0) = 0.254$ in that case.

3.3   The Fortran Code

The Fortran code which produces the illustrations of this paper is available on the web. Start at the author's homepage [8] `www.hep.fsu.edu/~berg` and follow the `research` and
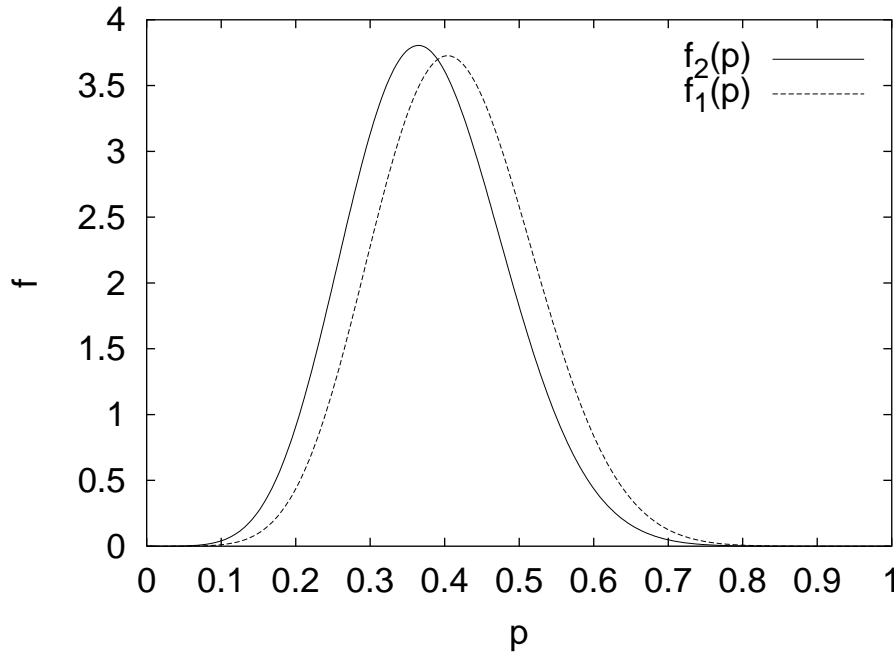

Figure 6: Probability densities $f_i(p)$ corresponding (14) to the cumulative distribution function of figure 4. The values used for N, N^Y, P_s and P_b are identical with those of figure 4.

from there the `Clopper-Pearson` hyperlink. Load down all files of the `Fortran Programs` subdirectory into an empty directory. Any standard Fortran 77 compiler should then be able to compile the `cp1.f`, `cp2.f` and `cp3.f` programs. Be aware that the program files include (via `include` Fortran statements) some of the other files you downloaded. Running one of the programs produces a data files with the name of that program and a `.d` extension. Subsequently, gnuplot users can produce the graphical presentations of this paper by using the `*.plt` driver files, as listed in the following.

```
    program           generates file          use with gnuplot driver

      cp1.f               cp1.d               cp1.plt

      cp2.f               cp2.d               cp2.plt, cp4.plt, cp5.plt, cp6.plt

      cp3.f               cp3.d               cp3.plt
```

Here, the gnuplot file number corresponds to the figure number of this paper. To get encapsulated postscript files, the comment signs in front of the first two rows of each gnuplot file have to be eliminated.

4   Conclusions

We have calculated confidence limits, and corresponding limits of the entire cumulative distribution function, for an unknown true signal likelihood p_{exact}. The only input used are the efficiencies P_s for tagging signals, the probabilities P_b for tagging background events, the number N^Y of tagged data and the total number of data N. In particular, the method allows to deal with the situation where only few signals occur and yields then a finite probability for the likelihood that $k \geq N^Y$ tags are observed if the true signal probability is $p_{\text{exact}} = 0$. In real life the probabilities P_s and P_b are most likely estimators by themselves, i.e. quantities with error bars. This causes no major problem, one just has to apply our confidence calculations to an appropriate sample and to average over the results.

References

[1] R.A. Fisher, Proc. Camb. Phil. Soc. 26, 528 (1930); Proc. Roy. Soc. A139, 343 (1933).

[2] J. Neyman and E.S. Pearson, Phil. Trans. Roy. Soc. A231, 289 (1933).

[3] C.J. Clopper and E.S. Pearson, Biometrika 26, 404 (1934). For a textbook treatment see S. Brandt, *Statistical and Computational Methods in Data Analysis* (North-Holland, 1983).

[4] B.A. Berg and J. Riedler, Comp. Phys. Commun. 107, 39 (1997).

[5] `http://alephwww.cern.ch/ALPUB/seminar/wds/`

[6] For the numerical evaluation of equations (9) use $\sum_{k=0}^{N} b_N^Y(k,p) = 1$ together with the partial sums from either $\sum_{k=N^Y}^{N} b_N^Y(k,p)$ or $\sum_{k=0}^{N^Y} b_N^Y(k,p)$, but not both. Normally $N^Y < N/2$ and $\sum_{k=0}^{N^Y} b_N^Y(k,p)$ will be used.

[7] B.A. Berg, *Introduction to Monte Carlo Simulations and Their Statistical Analysis*, in preparation.

[8] The address of the authors homepage and its tree structure are expected to be stable, whereas the absolute address where the programs are located is likely to change.